ACCESSORY PUBLICATION

Towards the Preparation of novel Re/99mTc Tricarbonyl-Containing

Peptide Nucleic Acid Bioconjugates

Gilles Gasser,^{A,*} Anna M. Sosniak,^B Anna Leonidova,^A Henrik Braband,^A and Nils Metzler-Nolte^{B,*}

^A Institute of Inorganic Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland.

^B Ruhr-University Bochum, Faculty of Chemistry and Biochemistry, Bioinorganic Chemistry Department I, Universitätsstrasse 150, D-44801 Bochum, Germany.

E-Mails: gilles.gasser@aci.uzh.ch; nils.metzler-nolte@rub.de

Table of contents

Figures S1 and S2: ¹ H- and ¹³ C-NMR spectra of Fmoc-4-O'Bu	2
Figures S3 and S4: ESI-MS and MALDI-TOF spectra of Dpam-PNA	3
Figure S5: LC-MS spectra of Dpam-PNA	4
Figure S6: ESI-MS of the methanolysis of [Re(CO) ₃ (3)]Br	4
Figure S7: MALDI-TOF spectrum of [Re(CO) ₃ (Fmoc-4-O ^t Bu)]Br	4
Figure S8: HPLC trace (γ detection) of the reaction of $[Tc(CO)_3(H_2O)_3]^+$ with Dpa'3HCl	5
Figure S9: HPLC trace (UV detection) of the Dpam-PNA solution	5



Figure S1. ¹H-NMR spectrum of Fmoc-4-O'Bu.



Figure S2. ¹³C-NMR spectrum of Fmoc-4-O^tBu.



Figure S3. ESI-MS spectrum of Dpam-PNA.



Figure S4. MALDI-TOF spectrum of Dpam-PNA.



Figure S5. HPL Chromatogram of Dpam-PNA.



Figure S6: ESI-MS of the methanolysis of $[Re(CO)_3(3)]Br$ with the isotopic pattern of $[Re(CO)_3(Dpa)]^+$ in insert.



Figure S7. MALDI-TOF spectrum of $[Re(CO)_3(Fmoc-4-O'Bu)]Br$ with the theoretical calculated isotopic pattern for C₄₆H₄₈N₈O₉Re $[M^+]$ in insert.



Figure S8. HPLC trace (γ detection) of the reaction of $[Tc(CO)_3(H_2O)_3]^+$ with **Dpa'3HCl** after 20 min at 95°C.



Figure S9. HPLC trace (UV detection) of the reaction of $[Tc(CO)_3(H_2O)_3]^+$ with **Dpam-PNA** after 60 min at 70°C.